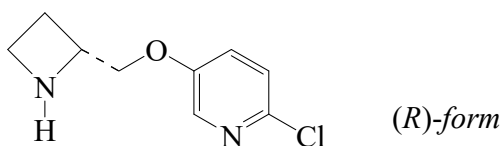




>>Entry Name: 5-(2-Azetidinylmethoxy)-2-chloropyridine, 9Cl

Synonym(s): ABT 594



Molecular Formula: C₉H₁₁ClN₂O

Molecular Weight: 198.651

Accurate Mass: 198.05599

Percentage Composition: C 54.42%; H 5.58%; Cl 17.85%; N 14.10%; O 8.05%

Biological Use/Importance: Potent , orally active non-opiate analgesic acting through neuronal nicotinic acetylcholine receptors

>>Variant: (R)-form

CAS Registry Number: 198283-73-7

Molecular Formula: C₉H₁₁ClN₂O

Molecular Weight: 198.651

Accurate Mass: 198.05599

Percentage Composition: C 54.42%; H 5.58%; Cl 17.85%; N 14.10%; O 8.05%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

CAS Registry Number: 203564-54-9

Melting Point: Mp 116-117°

Optical Rotation: [α]_D²³ +8.6 (c, 0.52 in MeOH)

>>Variant: (S)-form

CAS Registry Number: 203564-57-2

Molecular Formula: C₉H₁₁ClN₂O

Molecular Weight: 198.651

Accurate Mass: 198.05599

Percentage Composition: C 54.42%; H 5.58%; Cl 17.85%; N 14.10%; O 8.05%

>>Derivative: Hydrochloride (1:2)

CAS Registry Number: 203564-48-1

Extra CAS Registry Numbers(s): 203564-53-8

Melting Point: Mp 113-115°

References:

Holladay, M.W. *et al.*, *J. Med. Chem.*, 1998, **41**, 407-412, (*synth, pmr, pharmacol*)

Bannon, A.W. *et al.*, *Science (Washington, D.C.)*, 1998, **279**, 77-81, (*pharmacol*)